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OOPIC Simulation of a Cylindrical Magnetron Glow Discharge

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Abstract

An Object Oriented Particle-in-Cell model of a plasma glow discharge in a cylindrical magnetron cleaning device has been developed to provide guidance in developing a novel in situ surface conditioning technique. The model tracks the trajectories of particles by solving the equations of motion and the electrostatic field equations. Simulation results are compared to experimental measurements obtained from a plasma probe at 3 axial positions along the substrate surface.

1. INTRODUCTION

Adherent, erosion, and corrosion resistant coatings are critical to the performance of high performance armament systems. The U.S. Army Armament Research, Development, and Engineering Center's (ARDEC's) Benet Laboratories is currently developing a cylindrical magnetron sputtering (CMS) process for coating the bore of large caliber cannons to extend service life [1-2]. Benet is also developing a novel in situ plasma cleaning technique for conditioning the surface to promote adhesion of the sputter deposited coatings [3-4]. The plasma cleaning device (PCD) described in references 3 and 4 has been designed to etch both internal surfaces of a cylindrical magnetron system: the substrate and the sputter target. A schematic of the PCD with the glow discharge at the substrate cleaning section is illustrated in Figure 1. The operation of the substrate cleaning section is that of a hollow cathode device with the steel barrel serving as the cathode. The design of the PCD is being optimized using plasma simulation tools. Particle-in-Cell (PIC) techniques have been employed to simulate a DC glow discharge around the substrate cleaning section of the PCD. The PIC model computes the particle distribution as well as the energies of the ions for a mixture of Neumann and Dirichlet boundary conditions in a non-uniform magnetic field [5-6]. In this paper, the results from the simulations on the glow discharge near the internal surface of the barrel are compared to experimental data obtained from a retarding grid analyzer.

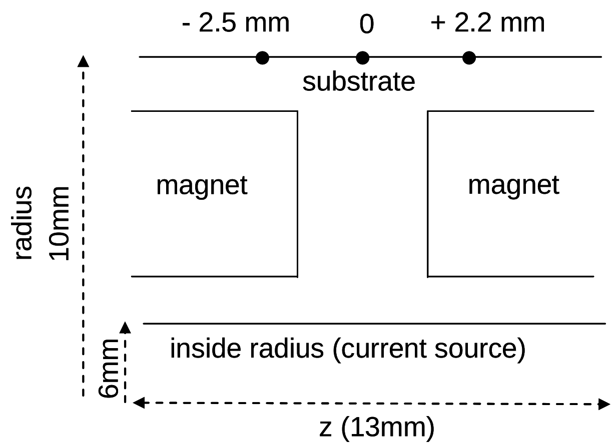

Figure 1. *Cross section of scaled PCD model.*

2. MODEL

A model of the PCD was developed using an object-oriented, 2½D (2d3v) plasma simulation code (OOPIC) developed by the Plasma Theory and Simulation Group at UC Berkeley [7]. PIC techniques model the interaction of primary electrons, secondary electrons, and ions with electric fields calculated based on charged particle locations. Computational constraints limit the particles in OOPIC simulations to a representative sampling of the properties of a much larger set of particles in real plasma. These macro-particles interact with fields defined on a grid (cells) and are interpolated to compute forces. The forces determine particle trajectories from integration of the Newton-Lorentz equations of motion. Particle collisions are incorporated into the simulation using Monte Carlo methods for the charged-particle, neutral collisions with energy dependent cross sections. The partial differential equations in OOPIC are solved using explicit finite difference methods and are therefore not unconditionally stable. The electromagnetic field equations are solved in OOPIC using an explicit finite difference time domain (FDTD) algorithm and particles are advanced using an explicit leap frog algorithm. Therefore, numerical stability requires a sufficiently small mesh size and time step.

The explicit FDTD solvers require the courant condition [8] be satisfied, which in 2 dimensions is given by:

$$c\Delta t\left(\frac{1}{\Delta r^2}+\frac{1}{\Delta z^2}\right)^{-1/2} \leq 1 \qquad (1)$$

where Δr and Δz are the mesh spacing in r and z, Δt is the time step, and *c* is the speed of light.

The leap-frog solver imposes additional constraints on Δt:

ω_{pe} Δt $\leq$ 2 for stability and ω_{pe} Δt $\leq$ 0.2 for accuracy [9], where $\omega_{pe} = \sqrt{\frac{n_e e^2}{\varepsilon_0 m_e}}$ is the electron plasma frequency, n_e is the electron density, *e* is the electron charge, m_e is the mass of an electron, and ε_0 is the permittivity of free space. Finite mesh stability also requires that $\Delta/\lambda_D < 1$, where λ_D is the Debeye length and Δ is the characteristic mesh spacing. This model assumes equilibrium charge densities n_e=n_i=n_0 so that λ_D is given by [9]:

$$\lambda_D = \sqrt{\frac{\varepsilon_0 T_e}{e n_0}} \qquad (2)$$

The scaled version of the PCD shown in figure 1 is employed because the stability criteria imposed practical limits on the size of the model that could be simulated with the available computational resources.

Gas breakdown is initiated by loading a uniform distribution of ions and electrons consistent with a low-density DC glow discharge. The fraction of ionization, n_i, in a low density discharge is on the order of $n_i = 10^{-5} n_g$, where n_g is the neutral gas density. This corresponds to 1.6e^{15} m^{-3} for the 5 mTorr model in this study. Therefore ω_{pe} is 2.3e^9 rad/s and Δt is limited to 80 ps. The initial electron temperature was set to T_{e0}= 5 eV and ion temperature to T_{i0}=0.035 eV. Scaling parameters were defined by mapping the PCD model to a 64x64 grid based on a cell size (Δ) limited to $\lambda_D/2$, or 200 μm. The magnetic fields associated with the permanent magnets was determined using FLUX2D [10], then fit to the OOPIC grid. The fields were scaled inversely proportional to the geometry to affect the same cyclotron orbits relative to the scaled geometry. The PCD model employs a radial current source derived from a simultaneous potential and circuit solution for two-dimensional simulation codes [11,12]. It was developed to address instability issues associated with the ideal voltage driven discharge in OOPIC. The instability is a consequence of gap impedance dropping as density increases, leading to positive feedback in current. The voltage source does not sag because it is ideal, therefore the power supplied to the plasma increases in proportion to the current. The magnitude of current source was set to 50 mA based on experimental determined current density of 56 A/m^2. The substrate and magnet pole faces were set to zero potential. This resulted in a steady state electrostatic potential that drops approximately 500 volts over the entire radial extent.

3. EXPERIMENT

The experimental cylindrical magnetron system described in references 1 and 2 is shown in Figure 2.

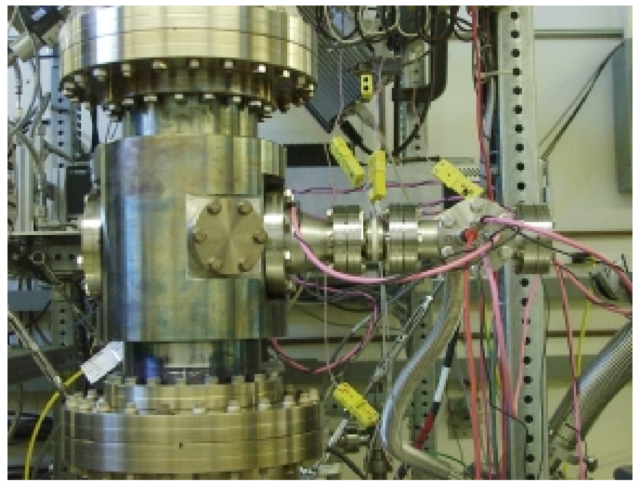

Figure 2. *Plasma probe encased inside conical flange; smaller flange of nipple was connected to a turbo pump-roughing vacuum system and the larger to the substrate chamber.*

The substrate surface in the form of a 120 mm inner diameter and 305 mm long cylinder was placed between two vacuum stacks. Argon, flowing at 2 sccm and regulated at 5 mT, was used as the background gas. The external surface of the PCD was 6.3 mm from the substrate (cathode) surface. The glow discharge was ignited around the substrate cleaning section, which is comprised of two conducting magnet pole faces and a collector. The potential of the anode surface for receiving the sputtered flux ranged from 250 to 300 volts. The magnet pole faces and the substrate were set at ground potential.

A retarding grid analyzer, or plasma probe, is a 25 mm long stainless steel cylinder with a 25mm outside diameter and contains a series of 4 grids and a current collector. Each grid is comprised of an electroformed nickel mesh inserted between two stainless steel washers. The mesh density is

118 lines/cm. The grids are electrically isolated using alumina disks. Details of the design of the plasma probe are given in references 13 and 14.

Figure 3 shows the installation of the plasma probe installed on the cylinder.

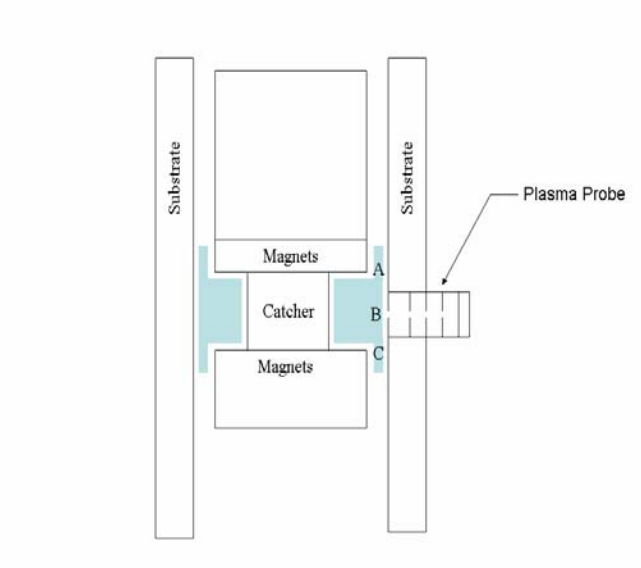

Figure 3. *Plasma Cleaning Device (PCD) showing substrate cleaning cross-section with shaded area representing the glow discharge. A = -2.5 mm, B = 0 mm, and C = +2.2 mm are positions of plasma probe aperture.*

The probe was mounted on the back of a 25 mm X 50 mm specimen with a surface that conformed to the internal surface of the cylinder. An orifice of 1.4 mm diameter was drilled on the conforming surface allowing charge particles impinging on the hole to be collected by the probe. The body and grid 1 of the probe were set at ground potential. Grid 2 was set at -10 volts to repel the electrons that passed through grid 1; grid 3 was the ion stopping voltage that varied between 0 and 600 volts; and finally, grid 4 and 5 were set at -50 and -40 volts respectively to prevent secondary electron current that resulted from ion bombardments at the collector from entering the collector. The probe was encased in an 11 cm to 7 cm conical reducer nipple as shown in figure 3.

The experimental data was collected using the plasma probe to determine the ion energy distribution at several locations along the substrate (the PCD was stationary at the selected locations). This approach entails applying increasing retarding voltages to the grid analyzer and measuring the ion current. Figure 4 shows the plots of current vs. voltage measurements at 3 PCD positions. The current at any voltage V is related to the ion energy distribution function $E(eV)$ by:

$$I(V) = A\int_{V}^{\infty} E(eV)dV \qquad (3)$$

where A is a constant. $E(eV)$ is proportional to the slope of the measured current as a function of the retarding potential. The ion energy distribution is obtained by differentiating the current with respect to voltage.

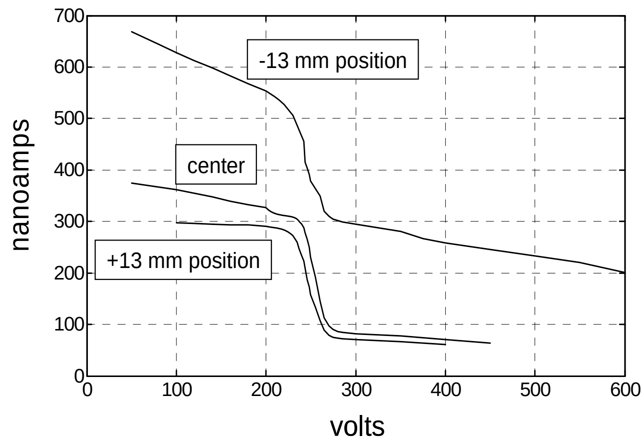

Figure 4. *Plasma probe measurements at 3 axial positions.*

4. SIMULATION RESULTS

Figure 5 shows that the solution reaches steady state in less than 3 microseconds. Stability was attained using a secondary emission coefficient of 0.5.

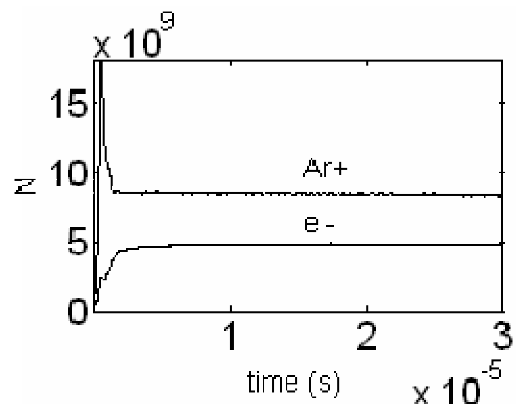

Figure 5. *Total number of argon ions, electrons, and secondary electrons vs. time.*

Figure 6 a-b-c shows the steady state particle distributions of the argon ions, electrons, and secondary electrons in z-r phase space after 30 microseconds. The cathode sheath at the substrate and magnet faces and anode sheath at the collector are apparent in the z-r space distribution for the electrons, which were generated from the ionization process. The substrate surface and the magnet pole faces, the ions and secondary electrons dominate the region indicating sputtering activity. The relatively low particle density of argon ions and secondary electrons at the magnet faces indicate a lower sputtering activity than at the substrate surface. This agrees with laboratory observation that the magnet pole faces receive a deposit from the substrate surface in spite of the argon ion bombardments.

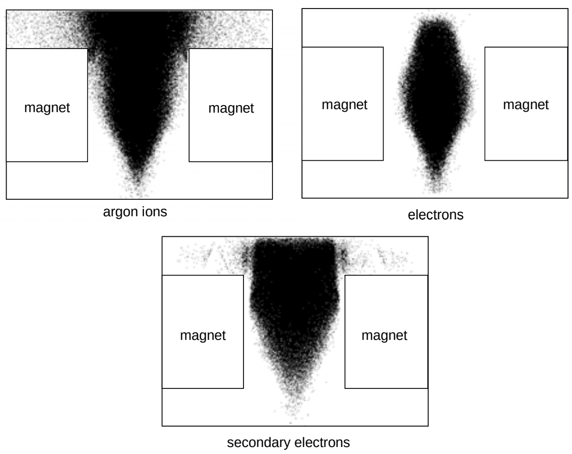

Figure 6. *Particle distributions in z-r space for a) argon ions; b) electrons from the ionization of argon neutrals by secondary electrons; c) secondary electrons emitted from the three ground conducting surfaces.*

5. COMPARISON OF SIMULATION AND EXPERIMENT

Figure 7 shows simulation results for the ion energy distribution at the surface. The origin of the bimodal distribution (25V and 200V peaks) is unclear, but it has been established that it is not a transient result.

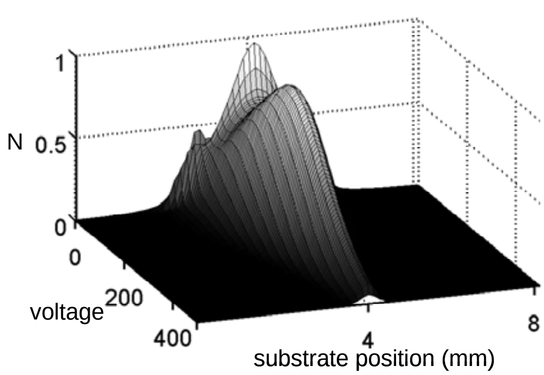

Figure 7. *Ion energy distribution determined by OOPIC simulation.*

Figure 8 shows a comparison of the simulation results with those calculated by differentiating with the I-V curves from figure 4. The distributions from the probe measurements show sharp peaks at 250 to 275 volts whereas the distributions from the simulation are very broad and centered around 200 volts. Simulation results for energies less than or greater than applied retarding voltages are excluded in the results. T(<100 volts) while the experimental data is again centered at 250 volts.

6. SUMMARY

Benet Laboratories is developing a novel in situ plasma cleaning technique for surface conditioning to promote adhesion of new erosion and corrosion resistant coatings for armament systems. Particle-in-cell simulation tools are being used as a means of providing guidance to engineers in the design of experimental systems in an effort to optimize this approach. We have successfully simulated a stable glow discharge using particle in cell simulation tools based on a model provided by the plasma theory and simulation group at U.C. Berkeley. A stable discharge was only attained using numerical parameters based on stability and accuracy constraints, not using parameters that exactly matched those of our system. Preliminary results are very encouraging, although the simulation has not yet reproduced the peaks observed in the particle energy distributions measured by a retarding grid analyzer at the 3 axial locations tested.

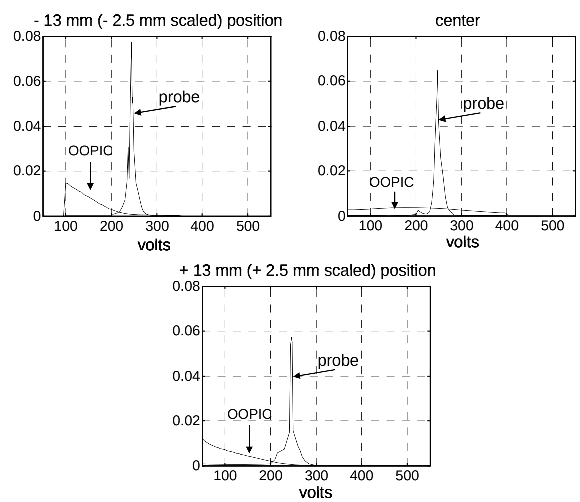

Figure 8. *Energy Distribution Function for ion energies determined using OOPIC and measured with plasma probe.*

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